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ABSTRACT

A simple pressure versus porosity compaction model is developed to calculate the response of granular porous bed materials to shock impact. The model provides a scheme for calculating compaction behavior when relatively limited material data is available. While the model was developed to study porous explosives and propellants, it has been applied to a much wider range of materials.

The early development of porous material models, such as that of Hermann,[1] required empirical dynamic compaction data. Erkman and Edwards[2] successfully applied the early theory to unreacted porous high explosives using a Gruneisen equation of state without yield behavior and without trapped gas in the pores. Butcher[3] included viscoelastic rate dependance in pore collapse. The theoretical treatment of Carroll and Holt[4,5] is centered on the collapse of a circular pore and includes radial inertia terms and a complex set of stress, strain and strain rate constitutive parameters. Unfortunately data required for these parameters are generally not available.

The model described here is also centered on the collapse of a circular pore, but utilizes a simpler elasto-plastic "static equilibrium" pore collapse mechanism without strain rate dependance, or radial inertia terms. It does include trapped gas inside the pore, a solid material flow stress that creates both a yield point and a variation in solid material pressure with radius. The solid is described by a Mie-Gruneisen type EOS. Comparisons show that this model will accurately estimate major mechanical features which have been observed in compaction experiments.

DESCRIPTION OF THE CALCULATION MODEL

Our model for the porous material is similar to previous models, a square array of equal sized spherical pores in a matrix of isotropic solid material, Figure 1. Macroscopic compression is resisted by (1) gas pressure inside each pore, (2) a spherical flow stress field centered about each pore, and (3) bulk compression of the matrix material which includes the thermal pressure. Required input data are simply the initial porosity, matrix material shock Hugoniot constants and the Gruneisen parameter value at full density, a matrix material yield stress, and initial values for pore gas pressure and temperature. The ratio between initial porous density and the solid theoretical maximum density (TMD) is referred to as the "density ratio". The "porosity" is then defined as the reciprocal of this density ratio.

The model is incorporated in a computer program which can produce a table of pressure versus cell deformation, and all deformation associated parameters such as porosity, compression, internal energy, gas conditions, etc. The program then reads the table, applies the conservation laws for mass and momentum and iterates to calculate the solution for the shock front conditions which gives values for particle velocity, shock front velocity, and pressure which of course can be compared to experimental data.

The elastic bulk modulus in general is a function of porosity and requires some special treatment. Kooker and Anderson[6] (KA) matched the acoustic data of Elban[7] on granular Teflon 7c, using an exponential function of porosity originally propounded for ceramics.[8] We use this KA function in the bulk modulus definition. Where the pressure is less than the yield point pressure, the calculated acoustic bulk velocity in porous material can be set close to that in material at theoretical maximum density (TMD), or less depending upon the function. The solid material bulk modulus is defined as the isentropic bulk modulus, a value that is estimated from the relationship of the Hugoniot pressure to the compression. The evaluation of the isentropic modulus $K = -v\left(\frac{\partial P}{\partial v}\right)_S$ can be obtained from the "Hugoniot modulus" $K_H = -v\left(\frac{\partial P}{\partial v}\right)_H$ if the Gruneisen parameter γ is known. (The equations are given in the appendix.)

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We have adopted the simplest (Von Mises) flow stress criteria. For the results illustrated here, it is assumed that matrix material plastic-flow stress (operating microscopically about each pore) is equal to the yield stress. Appropriate flow stress values have been obtained, for example, from high strain rate Hopkinson bar experiments. Alternatively, where shock Hugoniot yield data exist, an appropriate flow stress can be chosen to calculate a good fit to the experimental data.

Pressure and temperature rise in the pore gas is estimated from an ideal gas law. The gas compression constant, k, can be set for any assumed process behavior ranging from isothermal, $k = 1$, to isentropic, $k_{(s)} = C_p/C_v$. The results illustrated here assume air $k_{(s)} = 1.4$.

ANALYSIS

In the following, superscript "*" refers to the porous state and subscript "0" refers to the initial state. The subscript "1" identifies isothermal components and the subscript "2" identifies thermal components. No superscript indicates values for the matrix material. The porous material pressure, P^*, is described by a Mie-Gruneisen equation of state (EOS).

$$P^* = \phi_1(K^*, a, d, H, k) + \phi_2(G^*, u^*, E^*) \qquad (1)$$

The isothermal pressure, ϕ_1, is calculated as a function of compacting cell dimensions, a and d, bulk modulus, K^*, matrix material strength, H, and ideal gas flow pore gas process constant, k. The thermal pressure, ϕ_2, is calculated as a function of compaction cell geometry, porous material thermal energy E^*, and Gruneisen parameter, G^*.

The unit cell is a cube of matrix material with a centrally located spherical pore containing pore gas.

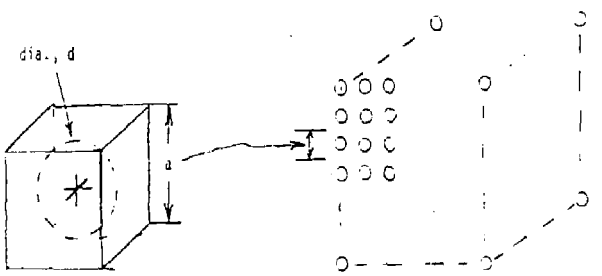


Figure 1.

Porosity, α, the ratio between total cell volume and the matrix volume, is computed from the cell-dimension, a, the matrix density, ρ, and initial values in porous cell density, ρ_0^*, and side length, a_0.

$$\alpha = \frac{\rho}{\rho_0^*} \times \left(\frac{a}{a_0}\right)^3 \qquad (2)$$

The pore diameter, d, is computed from the cell dimension and the porosity.

$$d = a\left[6/\pi\left(\frac{\alpha - 1}{\alpha}\right)\right]^{1/3} \qquad (3)$$

Porous material density, ρ^*, compression, μ^*, and relative volume V^* are defined.

$$\rho^* = \rho/\alpha \qquad (4)$$

$$\mu^* = \rho^*/\rho_0^* - 1 \qquad (5)$$

$$v^* = \rho_0^*/\rho^* \qquad (6)$$

Bulk Modulus

The porous material bulk modulus, K^*, is assumed to be a function of the porosity. Kooker related porous material acoustic velocity to matrix acoustic velocity

$$C_b^* = \exp\left(-C\frac{a-1}{a}\right) \cdot C_b \qquad (7)$$

The porous material bulk modulus is defined consistently with equations (7) and (8).

$$K^* = \left[\frac{1}{a}\exp\left(-2C\frac{a-1}{a}\right)\right] \cdot K \qquad (8)$$

The matrix material bulk modulus, K, increases with pressure, ϕ_1, as derived in equation (9) through (14). K is computed as an "isentropic" modulus. First, a "Hugoniot" modulus, K_H, is estimated at a Hugoniot point. It is defined as the derivative of the Hugoniot pressure, with compression.

$$K_H = \left[\frac{d\phi_1}{du}\right]_H \qquad (9)$$

Then with pressure given by,

$$\phi_1 = \rho_0 U_1 v \quad \text{and,} \qquad (10)$$

$$U_1 = C + S_1 v \qquad (11)$$

and the matrix material compression given by,

$$v = \rho/\rho_0 - 1 \qquad (12)$$

algebraic combination of equations (9) to (12) yield,

$$K_H = \frac{\rho_0}{C}(C + 2S_1 v)[C + (S_1 - 1)v]^2 \qquad (13)$$

where $v = \frac{C}{2S_1}\left[\sqrt{1 + \frac{4\phi_1 S_1}{\rho_0 C^2}} - 1\right]$

The isentropic bulk modulus can be obtained from the Hugoniot bulk modulus if the Grüneisen parameter is known; see appendix.

The result is $$K = K_H\left[1 - \frac{\gamma u}{2}\right] + \frac{\phi_1}{2}\,G \qquad (14)$$

Finally, the porous material isentropic bulk modulus, K*, is obtained from equations (8) and (14).

Elastic Deformation

Initially, all compaction cell deformation is bulk elastic deformation. The isothermal pressure is obtained by carrying out (stepwise) a path integral over the cell dimension, a.

$$\phi_1 = -3\int_{\text{elastic}} K^*(a,\alpha)\,\frac{d\alpha}{\alpha} \qquad (15)$$

The path is unique in the elastic regime and could in principal be derived in closed form. In this region, porosity and pore diameter are controlled by equations (2), (3), and (15).

In the plastic regime the path is not unique and must be carried out by iterative methods.

Plastic Flow

A volumetric average yield stress, $\sigma(k,H_y)$, equation (16), is calculated as the sum of the pore gas pressure and a matrix pressure that depends on the cell dimensions and the matrix uniaxial yield stress, $H = H_y$. The yield stress terms in equation (16) will be derived in equations (20) through (24). Small d, is pore diameter. For the cubic cell, volume a^3,

$$\underset{\text{cell}}{\sigma(k,H)} = \underset{\text{gas}}{P_0(\rho_0/d)^k} + \underset{\text{sphere}}{\alpha H\left(\frac{d}{a}\right)^3\left[\frac{1}{3}\left(\frac{e}{d}\right)^3\left(\ln\frac{a}{a_0} - \frac{1}{3}\right) + \frac{1}{9}\right]} + \underset{\text{curves}}{\left(2 - \frac{e}{3}\right)H\ln\frac{a}{a_0}} \qquad (16)$$

The gas compression process constant, k, can be any value equal to or larger than 1.0, which corresponds to an ideal isothermal process.

When ϕ_1 exceeds the yield stress from equation (16), the cell is assumed to flow plastically as well. In this regime, flow stress is calculated from equation (16) using a matrix flow stress, H = Hf, thus,

$$\phi_1 = s(k, H_f) \tag{17}$$

We assume that matrix flow stress equals matrix yield stress, i.e., HF = HY. Dimensional changes in a and d are computed incrementally as the sum of both bulk elastic deformation and constant volume flow deformation.

$$\delta a = \frac{a}{3K^*}\,\delta\phi_1 + \frac{\pi}{5}\left(\frac{d}{a}\right)^2 \delta d \tag{18}$$

Porosity and pore diameter now are controlled by equations (2), (3), and (18).

Compacted Elastic Deformation

During plastic flow, incremental elastic test pressures are evaluated.

$$\gamma = \phi_1\Big]_{N-1} - 3\,\frac{K^*\delta a}{a} \tag{19}$$

When this elastic calculation results in a lower pressure than the flow calculation from equation (17) for the same value of a, then the compaction process ceases to flow plastically. Thereafter the isothermal pressure is given by

$$\phi_1 = \gamma - 3\int_{\text{elastic}} K^* \frac{\delta a}{a} \tag{20}$$

where γ is the pressure where plastic flow ends. This criterion takes account of the fact that a pore can, in principal, be closed in a purely elastic fashion.

In this "locked up" elastic system, porosity and pore diameter are controlled by equations (2), (3), and (20).

Mechanical Pressure

The yield (flow) stress terms of equation (16) are based upon isotropic pore closing flow, at constant volume, in a spherical system with an origin at the center of the pore. The constant volume condition is expressed by,

$$\delta r^3 - d^3 = \delta r_0^3 - d_0^3 \tag{21}$$

"r" is a radius greater than the pore radius, d/2, but less than the compaction cell boundary of r = a/2. The equilibrium equation for a spherical element at, r, see Fig. 2, is

$$\left[p - \left(\frac{\partial p}{\partial r}\,\delta r\right) - p\right] r^2 d\theta^2 - 2Hr\delta r d\theta \frac{d\theta}{2} = 0.$$

When higher order differentials are dropped, the resultant pressure gradient equation is,

$$\frac{\partial p}{\partial r} = 2\frac{H}{r} \tag{22}$$

For pore gas pressure, p^*, and assuming that flow stress, H, does not vary with radius, the radial pressure at any radius less than r = a/2, but larger than r = d/2 is,

$$p(r) = p^* + 2H \ln\frac{2r}{d} \qquad , \qquad P_{max} = 2H \ln\frac{a}{d} \tag{23}$$

A mean volumetric pressure, s(r) is defined when equation (23) is integrated over the region circumscribed by radius r.

$$s(r) = \left[p^* r^3 + 6H \int_{d/2}^{r} r^2 \ln\frac{2r}{d}\, dr\right] \div r^3$$

After performing the integration to radius r = a/2, the result for the sphere, volume $\frac{\pi}{6} a^3$, is

$$\phi(a/2) = p^* + 6n \frac{d^3}{a^3}\left[\frac{a^3}{3d}\left(\ln\frac{a}{d} - \frac{1}{3}\right) + \frac{1}{9}\right] \tag{24}$$

Equation (24) yields a volumetric mean pressure in the sphere of diameter, a, within the compaction cell cube with side length, a. When the four corners of the superscribed cube are included at maximum pressure, the volumetric average expressed by equation (16) is the result.

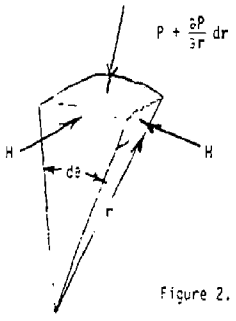


Figure 2.

Thermal Pressure

Thermal pressure, ϕ_2, is superposed after the isothermal pressure, ϕ_1, has been determined as a function of compaction geometry. The porous material Grueisen parameter, Γ^*, is assumed to be equal to the matrix parameter, G. The matrix parameter is reduced from the initial value using a density ratio.

$$\text{when } \rho^* < \rho_0 \quad , \quad G = G_0$$
$$\text{when } \rho^* > \rho_0 \quad , \quad G = \frac{\rho_0}{\rho^*} G_0 \tag{25}$$

Thermal pressure is given by

$$\phi_2 = \frac{\rho_0}{\rho^*} G_0 (1 + \mu^*) E^* \tag{26}$$

The thermal energy, E^*, is assumed to be the change in Hugoniot internal energy in the porous material minus the increase in the matrix isothermal energy.

$$E^* = \frac{1}{2}(1 + \mu^*) P^* - \int_0^{Q=P^*} \frac{Q}{K^*}\, dQ \tag{27}$$

The total pressure, P^*, is the sum of isothermal pressure, ϕ_1, and thermal pressure, ϕ_2.

Single Step Shock Hugoniot

A computer program creates a table of pressure versus cell deformation, and all deformation associated parameters such as porosity, compression, internal energy, gas conditions, etc. It then reads the table, applies the conservation laws for mass and momentum and iterates to calculate the solution for shock Hugoniot compaction front velocity and pressure rise for a steady "single step" wave traveling through a uniform porous material. All quantities are then plotted against particle velocity and compared to empirical data for compaction front velocity and pressure rise.

RESULTS

Equations of state for two different initial densities of porous pressed TNT[9] are illustrated in Figs. 3 and 4. The upper curve represents the total shock Hugoniot pressure. The bottom curve is the isothermal component. The asymptotic curve on the left is the isothermal pressure for the solid matrix material. The relative volume is 1.0 for the initial porous material. Unloading behavior can be modelled in various ways. A simple way that works well for most engineering purposes is illustrated in Figs. 6 and 7. Unloading occurs at a constant bulk modulus at a level that corresponds to the yield pressure and porosity when unloading begins.

Hugoniot compaction data exists for a wide range of materials. Figure 5 illustrates calculated versus experimental compaction velocity as a function of particle velocity for TNT. Figure 8 illustrates the compaction front pressure.

Variation in the value of the constant in the KA function (C in equation 8) changes the calculated constitutive behavior. This is illustrated for boron nitride[10] for C = 0., Fig. 9, C = 2.2, Fig. 10, and C = 5.0, Fig. 11. When C = 0 the material behaves as a rigid structural foam. When C = 2.2 the behavior will approximate the theoretical results of Carroll and Holt.[4] When C = 5.0 the material behaves in a very compliant fashion as in the experimental array of teflon balls. Figures 12, 13, and 14 show compaction front pressure versus particle velocity . . . corresponding to the constitutive behavior illustrated on Figs. 9, 10, and 11.

DISCUSSION

We have used a relatively simple material model to obtain a description of porous substances under compressive loading. We plan in the future to apply this model to the shock initiation of damaged explosives and to deflagation to detonation phenomenon.

As a practical matter most real materials are neither perfect aggregate nor perfect structural substances. Also, there is rather scant information on visco-plastic behavior of material, particularly on explosive materials.

Further, shock loading data in the region near yield is very scarce for all materials. A careful treatment of these two problems with special attention to the range of sensitivity of the results to the assumptions should be carried out before more sophisticated material behavior is incorporated in "compaction" models such as the one we have just reported.

Also, we make a plea here for more and better data on porous materials particularly in the yield stress regime where data is extremely scarce.

REFERENCES

1. Herrmann, W., "Constitutive Equations for the Dynamic Compaction of Ductile Porous Materials," J. Appl. Physics, 40 (. , 2490-2499 (1969).

2. Erkman, J.O., and Edwards, D. J., "Computed and Experimental Hugoniots in Unreacted Porous High Explosives," Pages 756 to 775, ACR-221, Office of Naval Research - Department of the Navy, 6th Symposium on Detonation, August 1976.

3. Butcher, B. M., "The Description of Strain-Rate Effects in Shocked Porous Materials," Shock Waves and the Mechanical Properties of Solids, (Syracuse University Press, Syracuse, New York, 1971), pp. 727-744.

4. Carroll, M. M., Holt, A. C., "Static and Dynamic Pore-Collapse Relations for Ductile Porous Materials," J. Appl. Physics, 43(4), 1626-1636 (1972).

5. Carroll, M. M., and Holt, A. C., "Suggested Modification of the P-Model for Porous Materials," J. Appl. Physics, 43 (2), 759-761 (1972).

6. Kooker, D. E. and Anderson, R. D., "A Mechanism for the Burning Rate of High Density, Porous, Energetic Materials," 7th Symposium on Detonation.

7. Elban, W. L., NSWC, unpublished data, 1980.

8. Knudsen, F. P., "Dependence of Mechanical Strength of Brittle, Polycrystalline Specimens on Porosity and Grain Size," J. Amer. Ceramic Soc., Vol. 42, No. 8, pp. 376-387, 1959.

9. Van Thiel, M., "Compendium of Shock Wave Data," UCRL 50108, 1967, Vol. 3, Data for TNT, 23-18-2-1(7-3-5-6)---1,7.

10. Van Thiel, M., "Compendium of Shock Wave Data," UCRL 50108, 1967, Vol. 2, Data for Boron-Nitride, 28-18---1,3.

APPENDIX

Fundamental thermodynamic equations of state definitions, combined with the Hugoniot jump conditions for change in internal energy, are used to relate isentropic bulk modulus, K, to Hugoniot bulk modulus K_H. First, five thermodynamic definitions are stated. I, is matrix energy per unit mass.

$$K_H = -V\left(\frac{\partial P}{\partial V}\right)_H \quad , \quad \text{Hugoniot bulk modulus} \tag{1}$$

$$K = -V\left(\frac{\partial P}{\partial V}\right)_S \quad , \quad \text{Isentropic bulk modulus} \tag{2}$$

$$G = V\left(\frac{\partial P}{\partial V}\right)_V \quad , \quad \text{Gruneisen value} \tag{3}$$

$$L = K/P \tag{4}$$

$$g = \frac{1}{P}\left(\frac{\partial I}{\partial V}\right)_P \tag{5}$$

The total differential energy identity is,

$$dI = \left(\frac{\partial I}{\partial V}\right)_P dV + \left(\frac{\partial I}{\partial V}\right)_V dP \tag{6}$$

Partial differentiations of (18) along an isentrope yields

$$\left(\frac{\partial I}{\partial V}\right)_S = \left(\frac{\partial I}{\partial V}\right)_P + \left(\frac{\partial I}{\partial V}\right)_V \left(\frac{\partial P}{\partial V}\right)_S \tag{7}$$

The relation for change in energy along an isentrope is,

$$\left(\frac{\partial I}{\partial V}\right)_S = -P \tag{8}$$

Equating (20) and (21) and substituting definitions (15) through (18) yields a thermodynamic identity.

$$g = \frac{L}{G} - 1 \tag{9}$$

The same procedure is now followed along the Hugoniot. Partial differentiation of (19) along the Hugoniot yields,

$$\left(\frac{\partial I}{\partial V}\right)_H = \left(\frac{\partial I}{\partial V}\right)_P + \left(\frac{\partial I}{\partial P}\right)_V \left(\frac{\partial P}{\partial V}\right)_H \tag{10}$$

The increase in internal energy across the Hugoniot shock limit is,

$$I = \frac{(P + P_o)}{2}(V_o - V) \tag{11}$$

Partial differentiation of (24) with respect to volume yields

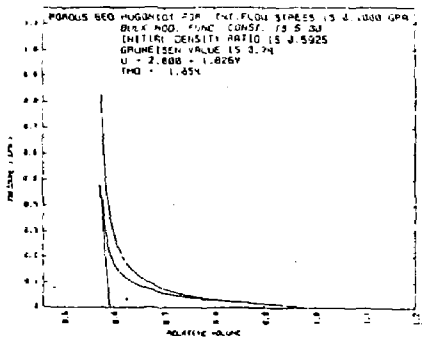
$$\left(\frac{\partial I}{\partial V}\right)_H = \frac{1}{2}\left(\frac{\partial P}{\partial V}\right)_H (V_o - V) - \frac{1}{2}(P + P_o) \tag{12}$$

Equating (23) and (25) and substituting in definitions 16 through 20 yield,

$$K = -GK_H\left[\frac{1}{2}\left(\frac{V_o}{V} - 1\right) - \frac{1}{G}\right] + \frac{(P + P_o)}{2} G \tag{13}$$

Since density is the reciprocal of specific volume, equation (12) can be combined with (26) leading to,

$$K = K_H\left[1 - \frac{uG}{2}\right] + \frac{(P + P_o)}{2} G \tag{14}$$



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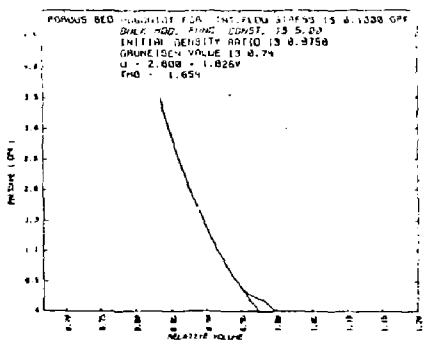

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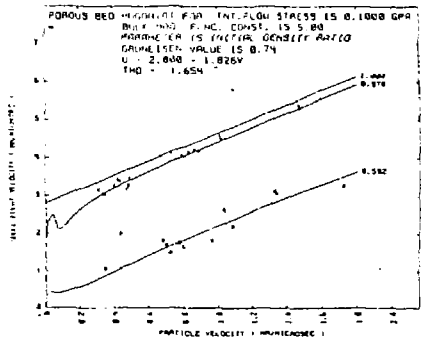

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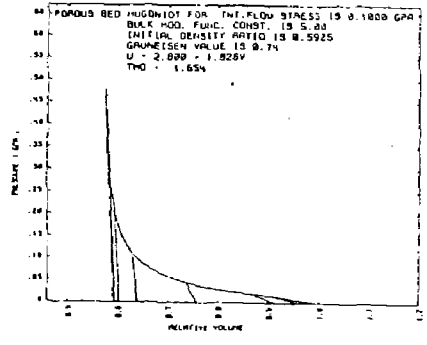

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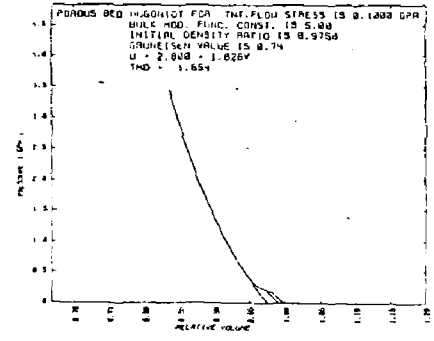

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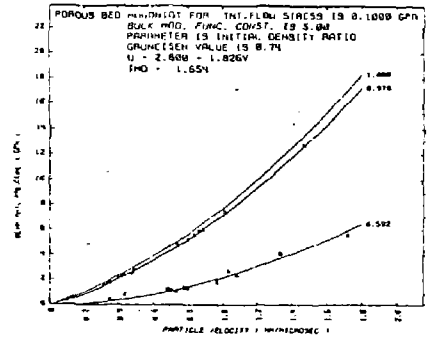

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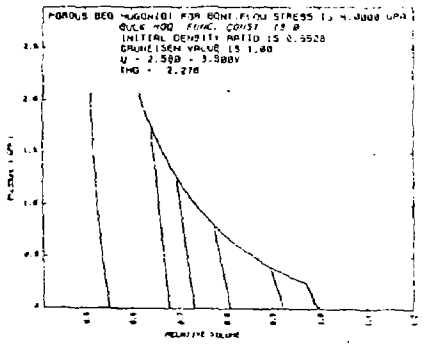

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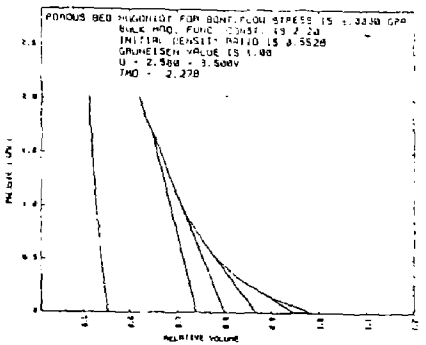

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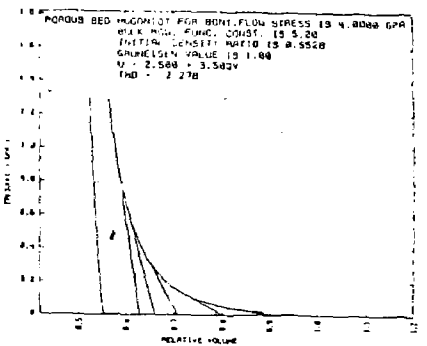

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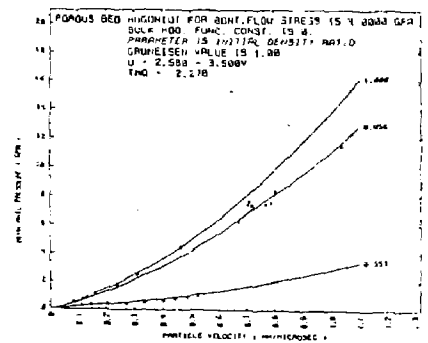

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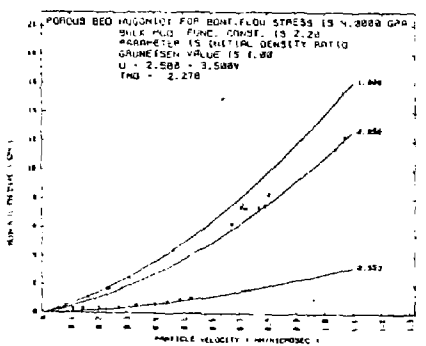

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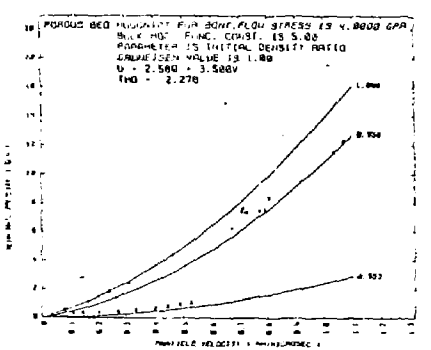

Figure 14